09/313048

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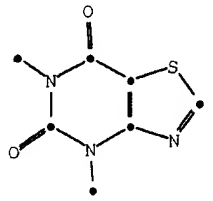

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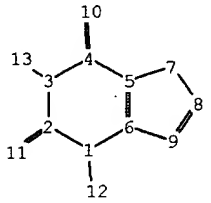

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10 11 12 13 14
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-12 2-11 3-13 4-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
1-2 1-6 1-12 2-3 2-11 3-4 3-13 4-5 4-10 5-6 5-7 6-9 7-8
8-9

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS

FILE 'REGISTRY' ENTERED AT 10:25:07 ON 21 SEP 1999
L1 STRUCTURE UPLOADED
L2 1 S L1

FILE 'REGISTRY' ENTERED AT 10:40:51 ON 21 SEP 1999
L3 STRUCTURE UPLOADED
L4 1 S L3
L5 27 S L3 FULL SSS

FILE 'CAPLUS' ENTERED AT 10:41:48 ON 21 SEP 1999

=> s l5

L6 11 L5

=> d l6 ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 11 ANSWERS - CONTINUE? Y/(N):y

L6 ANSWER 1 OF 11 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1994:456825 CAPLUS
DOCUMENT NUMBER: 121:56825
TITLE: Iminoethenethiones, RN:C:C:S: Characterization by Neutralization-Reionization Mass Spectrometry and G2(MP2) Theory
AUTHOR(S): Flammang, Robert; Landu, Dinzeyi; Laurent, Sophie; Barbieux-Flammang, Monique; Kappe, C. Oliver; Wong, Ming Wah; Wentrup, Curt
CORPORATE SOURCE: Department of Organic Chemistry, University of MonsHainaut, Mons, B-7000, Belg.
SOURCE: J. Am. Chem. Soc. (1994), 116(5), 2005-13
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

QD1 A5

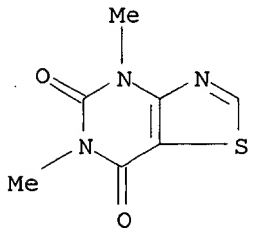
AB (Methylimino)ethenethione (2) and iminoethenethione (4) are stable mols. on the microsecond time scale of neutralization-reionization mass spectrometry expts. The corresponding radical cations were generated by fragmentation of thiazolopyrimidinedione mol. ions. Iminoethenethione (4) does not tautomerize to thioformyl cyanide (HCSCN) under the wall-less conditions of the MS expt., but it does so under FVP conditions when generated from isoxazolones. Thioformyl cyanide was unequivocally identified by IR and mass spectra. The structures and stabilities of 2, 4, and 4.bul.+ were investigated by ab initio calcns. at the G2(MP2) level of theory. Both 2 and 4 are predicted to have a singlet ground state, in contrast to O:C:C:S, for which a triplet state is preferred. The singlet-triplet gaps are approx. 40 kJ mol-1. In agreement with exptl. findings, both iminoethenethiones are calcd. to be thermodynamically and kinetically stable species, lying in energy wells with at least a 100 kJ mol-1 barrier to dissocn. into HNC (or CH3NC) + CS. The IR and UV spectra and ionization energies of 2 and 4 are predicted. The iminoethenethione radical cation (4.bul.+) is found to be the global min. on the C2HNS.bul.+

potential energy surface and stable toward all possible fragmentations: the most favorable fragmentations into H.bul. + NCCS+ and HNC + CS.bul.+ are in accord with the mass spectrometric observations.

IT **1781-18-6**
RL: RCT (Reactant)
(characterization of iminoethenethiones by neutralization-reionization mass spectrometry of heterocycles)

RN 1781-18-6 CAPLUS

CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L6 ANSWER 2 OF 11 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1988:179589 CAPLUS

DOCUMENT NUMBER: 108:179589

TITLE: Non-xanthine heterocycles: activity as antagonists of A1- and A2-adenosine receptors

AUTHOR(S): Daly, John W.; Hong, Oksoon; Padgett, William L.; Shamim, Mah T.; Jacobson, Kenneth A.; Ukena, Dieter

CORPORATE SOURCE: Lab. Chem. Bioorg. Chem., Natl. Inst. Diabetes, Dig. Kidney Dis., Bethesda, MD, 20892, USA

SOURCE: Biochem. Pharmacol. (1988), 37(4), 655-64
CODEN: BCPCA6; ISSN: 0006-2952

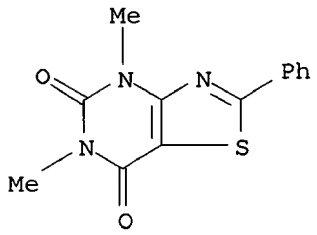
DOCUMENT TYPE: Journal

LANGUAGE: English

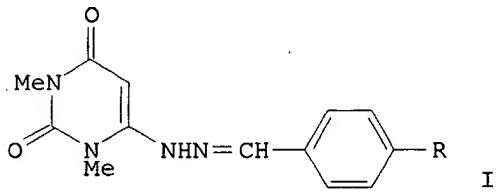
AB A variety of nonxanthine heterocycles were antagonists of binding of [3H]phenylisopropyladenosine to rat brain A1-adenosine receptors and of activation of adenylate cyclase via interaction of N-ethylcarboxamidoadenosine with A2-adenosine receptors in human platelet and rat pheochromocytoma cell membranes. The pyrazolopyridines tracazolate, cartazolate, and etazolate were several fold more potent than theophylline at both A1- and A2-adenosine receptors. The pyrazolopyridines, however, were still many fold less potent than 8-phenyltheophylline and other 8-phenyl-1,3-dialkylxanthines. A structurally related N6-substituted 9-methyladenine was also a potent adenosine antagonist with selectivity for A1 receptors. None of several aryl-substituted heterocycles, including a thiazolopyrimidine, imidazopyridines, benzimidazoles, a pyrazoloquinoline, a mesoionic xanthine analog, and a triazolopyridazine exhibited the high potency typical of 8-phenyl-1,3-dialkylxanthines. A furyl-substituted triazoloquinazoline was very potent at both A1 and A2 receptors. A pteridin-2,4-dione, 1,3-dipropyllumazine, was somewhat less potent than theophylline at A1- and A2-adenosine receptors, whereas 1,3-dimethyllumazine was much less potent. A benzopteridin-2,4-dione, alloxazine, was somewhat more potent than theophylline. Other heterocycles with antagonist activity were the dibenzazepine carbamazepine and .beta.-carboline-3-Et carboxylate. The phenylimidazoline clonidine had no activity, whereas a related dihydroxyphenylimidazoline was a weak noncompetitive adenosine antagonist.

IT **21544-68-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and as adenosine receptor antagonist, structure in relation to)

RN 21544-68-3 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl-2-phenyl- (8CI, 9CI) (CA INDEX NAME)

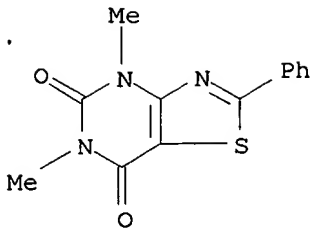


L6 ANSWER 3 OF 11 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1985:615258 CAPLUS
DOCUMENT NUMBER: 103:215258
TITLE: Reaction of 6-arylidenehydrazino-1,3-dimethyluracils with thionyl chloride leading to purine, thiazolo[4,5-d]pyrimidine, pyrimido[4,5-e][1,3,4]thiadiazine, pyrazolo[3,4-d]pyrimidine, and [1,2,3]thiadiazolo[4,5-d]pyrimidine derivatives
AUTHOR(S): Ichiba, Misuzu; Senga, Keitaro
CORPORATE SOURCE: Sch. Med., Keio Univ., Tokyo, 160, Japan
SOURCE: J. Heterocycl. Chem. (1985), 22(2), 381-4
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:215258
GI

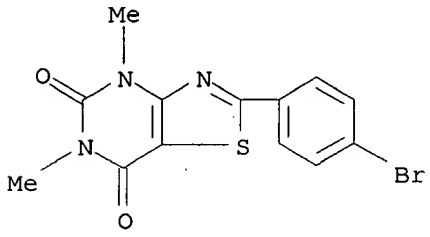


I

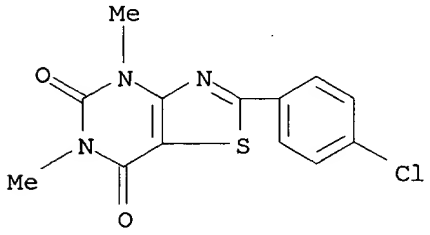
AB The reaction of 6-arylidenehydrazino-1,3-dimethyluracils I (R = H, Br, Cl, Me, OMe) with SOCl2 in C6H6 afforded purine, thiazolo[4,5-d]pyrimidine, pyrimido[4,5-e][1,3,4]thiadiazine, pyrazolo[3,4-d]pyrimidine, and [1,2,3]thiadiazolo[4,5-d]pyrimidine derivs. The treatment of 6-(benzylidene-1'-methylhydrazino)-1,3-dimethyluracil with SOCl2 in C6H6 gave 4-methylpyrimido[4,5-d][1,3,4]thiadiazine and 1-methylpyrazolo[3,4-d]pyrimidine derivs. Plausible mechanisms for the formation of these fused pyrimidines are discussed.
IT **21544-68-3P 99261-90-2P 99261-91-3P 99261-92-4P 99261-93-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 21544-68-3 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl-2-phenyl- (8CI, 9CI) (CA INDEX NAME)



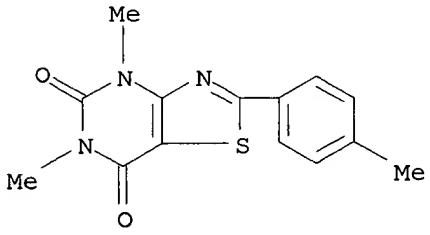
RN 99261-90-2 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 2-(4-bromophenyl)-4,6-dimethyl- (9CI) (CA INDEX NAME)



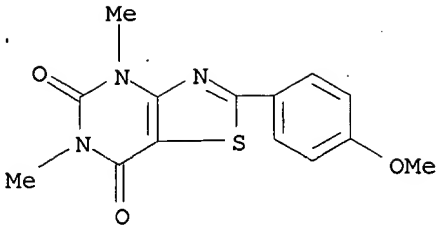
RN 99261-91-3 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 2-(4-chlorophenyl)-4,6-dimethyl- (9CI) (CA INDEX NAME)



RN 99261-92-4 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 99261-93-5 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 2-(4-methoxyphenyl)-4,6-dimethyl- (9CI) (CA INDEX NAME)



L6 ANSWER 4 OF 11 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1985:6061 CAPLUS
DOCUMENT NUMBER: 102:6061
TITLE: Antagonists for adenosine receptors
INVENTOR(S): Snyder, S. H.; Daly, J. W.; Bruns, R. F.
PATENT ASSIGNEE(S): John Hopkins University, USA
SOURCE: Belg., 39 pp.
CODEN: BEXXAL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 898946	A1	19840618	BE 1984-212418	19840217
US 4593095	A	19860603	US 1983-467894	19830218
SE 8400788	A	19840819	SE 1984-788	19840214
SE 456680	B	19881024		
SE 456680	C	19890216		
FR 2541281	A1	19840824	FR 1984-2472	19840217
FR 2541281	B1	19880129		
GB 2135311	A1	19840830	GB 1984-4243	19840217
GB 2135311	B2	19861105		
NL 8400514	A	19840917	NL 1984-514	19840217
DE 3406275	A1	19840927	DE 1984-3406275	19840217
CA 1234804	A1	19880405	CA 1984-447705	19840217
JP 59205377	A2	19841120	JP 1984-28010	19840218
US 4769377	A	19880906	US 1986-825594	19860203
PRIORITY APPLN. INFO.:			US 1983-467894	19830218

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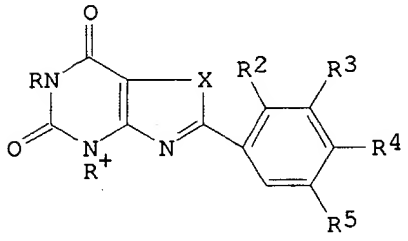

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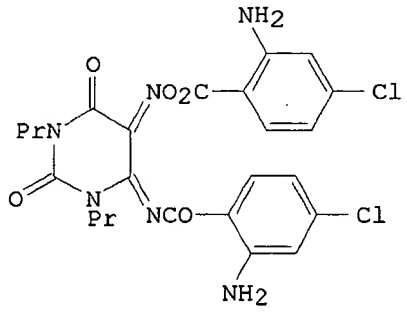


II

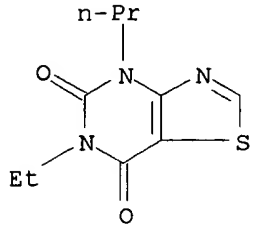
AB Xanthine derivs. I [X = NH, O, S; R = allyl, (un)substituted alkyl, cycloalkyl; R1 = H, allyl, (un)substituted alkyl, cycloalkyl; R2 = NH2, OH; R3, R5 = H, halogen, alkyl, alkoxy, OH, NO2, NH2; R4 = halogen, (un)substituted alkyl, Ph, amino, cycloalkyl, OH, CO2H, alkoxy, cycloalkoxy] were prepd. Thus 4,2-Cl(O2N)C6H3CO2H were treated with 1,3-dipropyl-5-nitroso-6-aminouracil and the resulting diimine II reduced with (NH4)2S to give I (X = NH, R = R1 = Pr; R2 = NH2, R3 = R5 = H, R4 = Cl, III). III had a cyclohexyladenosine antagonist ED50 of 0.05 nM in

vitro. Cyclohexyladenosine antagonist data are give for >90 I and structure-activity relationships are discussed.

IT **3758-26-7**
RL: RCT (Reactant)
(adenosine antagonist activity of)

RN 3758-26-7 CAPLUS

CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 6-ethyl-4-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L6 ANSWER 5 OF 11 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1981:435269 CAPLUS

DOCUMENT NUMBER: 95:35269

TITLE: Adenosine antagonism by purines, pteridines, and benzopteridines in human fibroblasts

AUTHOR(S): Bruns, Robert F.

CORPORATE SOURCE: Dep. Neurosci., Univ. California, La Jolla, CA, 92093, USA

SOURCE: Biochem. Pharmacol. (1981), 30(4), 325-33
CODEN: BCPCA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

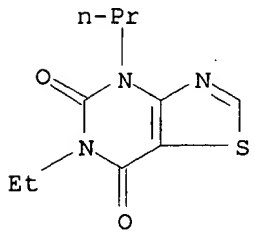
Q09 01
B5

AB Testing of >100 purine bases and structurally related heterocycles as adenosine (I) [58-61-7] antagonists in VA13 fibroblasts (detd. by cAMP increase) yielded 3 families of I antagonists: xanthines, benzo[g]pteridines, and 9-substituted adenines. For the xanthines, the optimal group at the 1-position was Bu (5-fold improvement vs. Me), at the 7-position was 2-chloroethyl (5-fold improvement vs. H), and at the 8-position was p-bromophenyl (100-fold improvement vs. H). The receptors apparently had butyl- and phenyl-sized pockets at the 1- and 8-positions, resp., since compds. with larger groups had greatly reduced activity.

IT **3758-26-7**
RL: BIOL (Biological study)
(adenosine receptor of fibroblast antagonism by)

RN 3758-26-7 CAPLUS

CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 6-ethyl-4-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L6 ANSWER 6 OF 11 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1980:22750 CAPLUS

DOCUMENT NUMBER: 92:22750

TITLE: Studies on heterocyclic compounds. Part XXIX. A one-step synthesis of glycosylaminoisothiazolo[3,4-d]pyrimidines and glycosylaminoisothiazoles

AUTHOR(S): Takahashi, Hiroshi; Nimura, Noriyuki; Ogura, Haruo
CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan

SOURCE: Chem. Pharm. Bull. (1979), 27(5), 1147-52
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English

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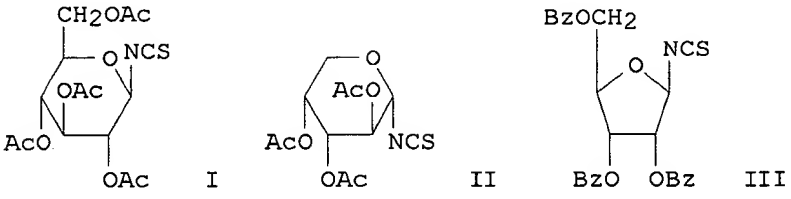
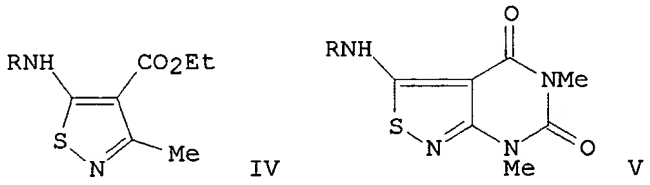
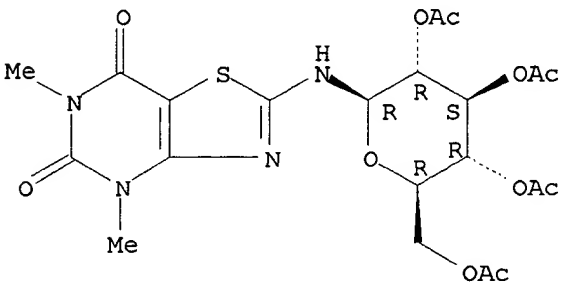




AB The reaction of glycosyl isothiocyanate I with 2-aminopyridine or 2-amino-4-picoline gave N-glycosyl-N'-(2-pyridyl) thiourea and N-glycosyl-N'-(4-methyl-2-pyridyl) thiourea, resp., in good yields; cyclized products were not obtained. On the other hand, the reaction of glycosyl isothiocyanates I, II, and III with MeC(NH2):CHCO2Et gave MeC(NH2):C(CSNHR)CO2Et (R = glycosyl) and nucleoside analogs IV (R = glycosyl). Similar reaction of I-III with 6-amino-1,3-dimethyluracil gave nucleoside analogs V.

IT **71399-40-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 71399-40-1 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 2,3-dihydro-4,6-dimethyl-2-[(2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranosyl)imino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 7 OF 11 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1974:48027 CAPLUS

DOCUMENT NUMBER: 80:48027
TITLE: Thiazolopyrimidines by reaction of 6-amino-1,3-dimethyluracil with alkyl isothiocyanate
INVENTOR(S): Berger, Arthur; Borgaes, Edeltraut E.
PATENT ASSIGNEE(S): Baxter Laboratories, Inc.
SOURCE: U.S., 4 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3772290	A	19731113	US 1971-200208	19711118
US 3660405	A	19720502	US 1969-849899	19690813
GB 1285268	A	19720816	GB 1970-1285268	19700729
US 3745217	A	19730710	US 1971-200209	19711118
US 3769287	A	19731030	US 1971-200207	19711118

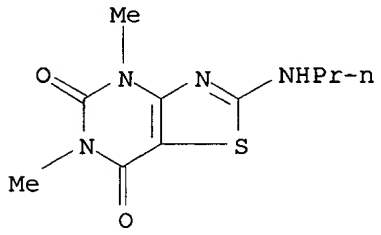
PRIORITY APPLN. INFO.: US 1969-849899 19690413

GI For diagram(s), see printed CA Issue.

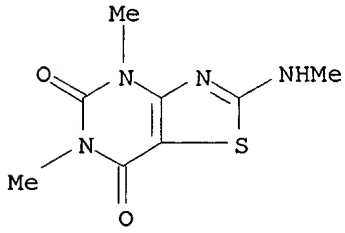
AB Thiazolopyrimidines I (R = Me, Et, Pr, Bu, allyl) were prepd. by cyclizing 6-amino-1,3-dimethyluracil with RNCS or by cyclizing the corresponding pyrimidinylthiourea with Br or H2O2. I had a barbiturate antagonist ED50 of 7.2-49 mg/kg i.p. in mice at LD50/ED50 ratios of 2.95-73.6.

IT **31894-92-5P 31894-93-6P 31895-48-4P 31895-49-5P 31895-50-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

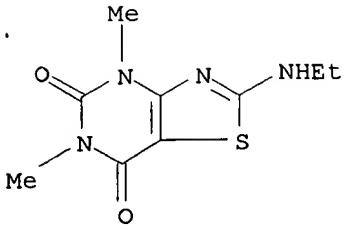
RN 31894-92-5 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl-2-(propylamino)-(9CI) (CA INDEX NAME)



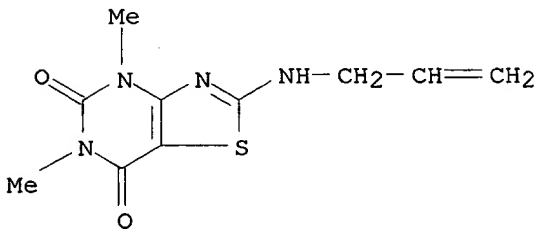
RN 31894-93-6 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl-2-(methylamino)-(9CI) (CA INDEX NAME)



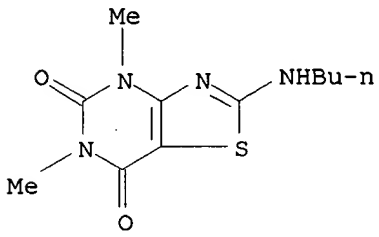
RN 31895-48-4 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 2-(ethylamino)-4,6-dimethyl-(9CI) (CA INDEX NAME)



RN 31895-49-5 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl-2-(2-propenylamino)- (9CI) (CA INDEX NAME)



RN 31895-50-8 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 2-(butylamino)-4,6-dimethyl-(9CI) (CA INDEX NAME)

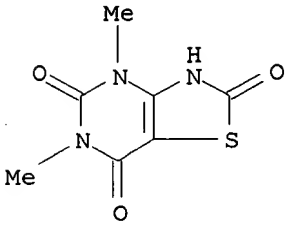


L6 ANSWER 8 OF 11 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1974:37148 CAPLUS
DOCUMENT NUMBER: 80:37148
TITLE: Fungicidal thiazolo[4,5-d]pyrimidines
INVENTOR(S): Grohe, Klaus
PATENT ASSIGNEE(S): Bayer A.-G.
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

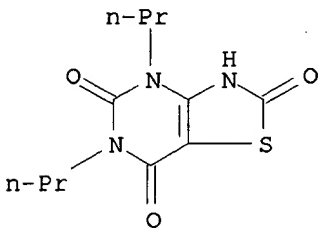
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2223421	A1	19731122	DE 1972-2223421	19720513

GI For diagram(s), see printed CA Issue.
AB Four thiazolopyrimidines I (R = CH2Ph or H; R1 = Me, Pr, or CH2-CN2Ph) were prepd. in 54-86% yield by reaction of the aminouracil II with ClCOSCl in PhCl with subsequent heating. I (R = H, R1 = Me) had fungicidal activity in rice cultures.
IT **49679-82-5P 49679-83-6P 49679-84-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

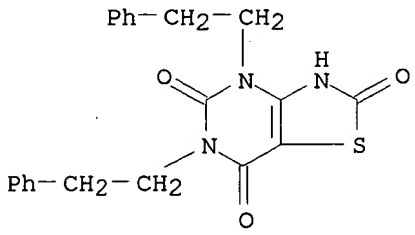
RN 49679-82-5 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-2,5,7(3H,4H,6H)-trione, 4,6-dimethyl- (9CI) (CA
INDEX NAME)



RN 49679-83-6 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-2,5,7(3H,4H,6H)-trione, 4,6-dipropyl- (9CI) (CA
INDEX NAME)



RN 49679-84-7 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-2,5,7(3H,4H,6H)-trione, 4,6-bis(2-phenylethyl)-
(9CI) (CA INDEX NAME)

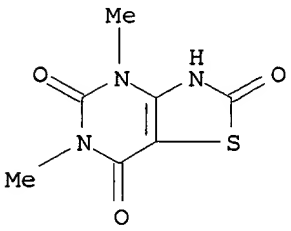


L6 ANSWER 9 OF 11 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1973:478673 CAPLUS
DOCUMENT NUMBER: 79:78673
TITLE: Cycloacylation of enamines. I. Synthesis of 2-thiazolone derivatives
AUTHOR(S): Grohe, Klaus; Heitzer, Helmut
CORPORATE SOURCE: Wiss. Hauptlab., Bayer A.-G., Leverkusen, Ger.
SOURCE: Justus Liebigs Ann. Chem. (1973), (5-6), 1018-24
CODEN: JLACBF
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB Cycloacylation of the enamines RNHCR2:CHCO2R1, RO2CCH:CMeNHZNHCMe:CHCO2R, MeNHCMe:CHCONHR, RNHCMe:CHCN, and 4-O2NC6H4CH:C(NH2)C6H4NO2-4 with ClCOSCl gave the thiazolones I (R = H, Me, Ph, CH2Ph; R1 = C1-12 alkyl, cyclohexyl, PhCH2, or PhCH2CH2; R2 = Me, CCl3, or CO2Et), II (R = Me or Et, Z = CH2CH2 or p-C6H4), III [R = Ph or 4,3,6-Cl(MeO)2C6H2], IV (R = H,

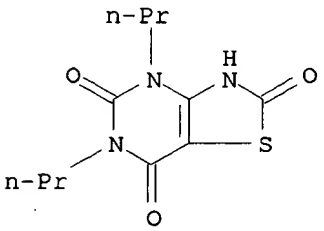
PhCH2, Ph, 3-ClC6H4, or 3-MeC6H4) and V, resp. Reaction of the uracils VI
with ClCOSCl gave the thiazolopyrimidines VII (R = Me, Pr, or PhCH2CH2, R1
= H or PhCH2).

IT **49679-82-5P 49679-83-6P 49679-84-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

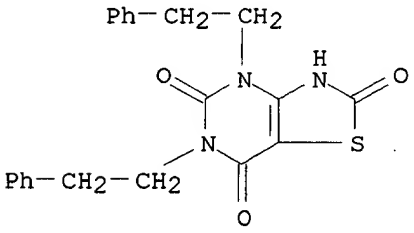
RN 49679-82-5 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-2,5,7(3H,4H,6H)-trione, 4,6-dimethyl- (9CI) (CA
INDEX NAME)



RN 49679-83-6 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-2,5,7(3H,4H,6H)-trione, 4,6-dipropyl- (9CI) (CA
INDEX NAME)



RN 49679-84-7 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-2,5,7(3H,4H,6H)-trione, 4,6-bis(2-phenylethyl)-
(9CI) (CA INDEX NAME)



L6 ANSWER 10 OF 11 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1970:12658 CAPLUS
DOCUMENT NUMBER: 72:12658
TITLE: Reactions of 6-amino-1,3-dimethyluracils with thionyl chloride. I. Novel thiazole synthesis. 4,5,6,7-Tetrahydrothiazolo[4,5-d]pyrimidine-5,7-diones
AUTHOR(S): Goldman, Irving M.
CORPORATE SOURCE: Med. Res. Lab., Chas. Pfizer and Co., Inc., Groton, Conn., USA

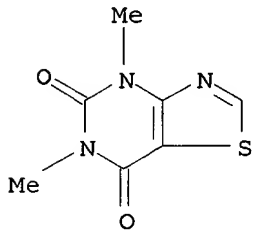
SOURCE: J. Org. Chem. (1969), 34(11), 3285-9
CODEN: JOCEAH
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

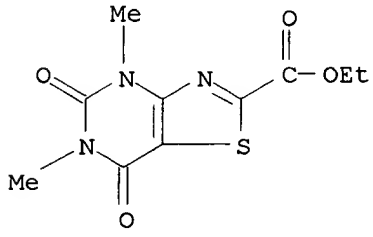
AB 6-Amino-1,3-dimethyluracils (I, R = H, CO2H, CO2Et, Ph, and CF3) undergo facile conversion to the corresponding thiazolopyrimidines (II) upon treatment with SOCl2-pyridine, except for I (R = CF3), where SOCl2 is more effective in absence of pyridine. II (R = H, CO2H and CO2Et) were reported previously by Schroeder(1964). The reaction is presumed to proceed via dehydration of the intermediate thiazoline S-oxides. A different reaction is observed when an inferior grade of SOCl2 is use d in the absence of pyridine, resulting in the formation of sulfides and p roducts derived therefrom. Speculation is offered on the mechanism of thiazole formation from suitably substituted 6-aminouracils.

IT **1781-18-6P 3764-04-3P 21544-68-3P**
21544-69-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

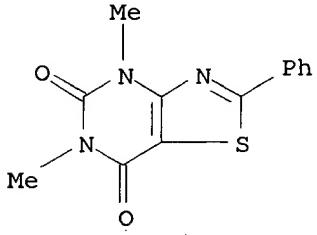
RN 1781-18-6 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



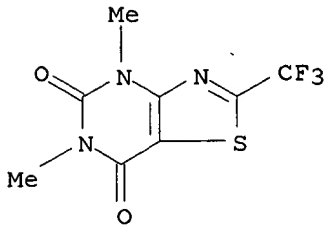
RN 3764-04-3 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-2-carboxylic acid, 4,5,6,7-tetrahydro-4,6-dimethyl-5,7-dioxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



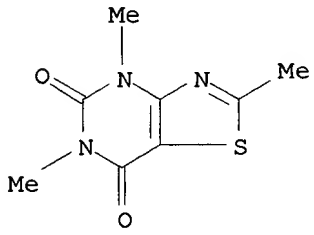
RN 21544-68-3 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl-2-phenyl- (8CI, 9CI) (CA INDEX NAME)



RN 21544-69-4 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl-2-(trifluoromethyl)- (8CI) (CA INDEX NAME)



L6 ANSWER 11 OF 11 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1968:436067 CAPLUS
DOCUMENT NUMBER: 69:36067
TITLE: Thiazolo-N-hydroxyuracils
AUTHOR(S): Bauer, Ludwig; Mahajanshetti, C. S.
CORPORATE SOURCE: Med. Center, Univ. of Illinois, Chicago, Ill., USA
SOURCE: J. Heterocycl. Chem. (1968), 5(3), 331-5
CODEN: JHTCAD
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The partial Lossen degradation of the hydroxamic acid group at C-4 of C-5 of Na 4,5-thiazoledicarbohydroxamate and its 2-Me analog initiated a multicoursed reaction which furnished a mixt. of thiazolo[4,5-d]- (I) and thiazolo[5,4-d]-N-hydroxyuracils (II). The isomer distribution was sensitive to the solvent systems in which these reactions were carried out. The structure of the isomers so obtained was established by chem. and spectral methods.
IT **18903-27-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 18903-27-0 CAPLUS
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 2,4,6-trimethyl- (8CI) (CA INDEX NAME)



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L5            27 S L3 FULL SSS

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     FILE 'STNGUIDE' ENTERED AT 10:42:56 ON 21 SEP 1999

     FILE 'CAOLD' ENTERED AT 10:49:54 ON 21 SEP 1999


=> s l5

L7             4 L5

=> d ibib ab hitstr 1-
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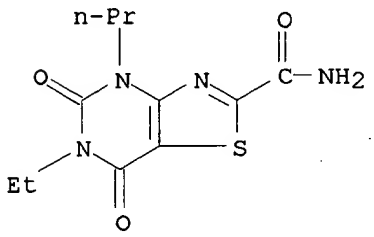
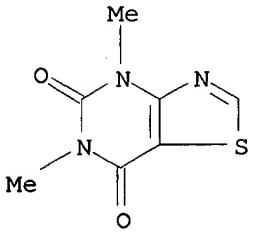
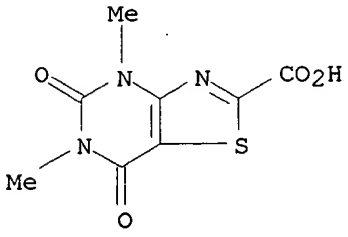
L7 ANSWER 1 OF 4 CAOLD COPYRIGHT 1999 ACS
ACCESSION NUMBER: CA62:4036e CAOLD
TITLE: 4,6-dialkyl-5,7-dioxothiazolo[4,5-d]pyrimidine-2-carboxylic acid and derivs.
AUTHOR NAME: Schroeder, Elmer F.
DOCUMENT TYPE: Patent
TITLE: 4,6-dialkyl-5,7-dioxothiazolo[4,5-d]pyrimidine-2-carboxylic acid and derivs.
PATENT ASSIGNEE: Searle, G. D., & Co.
DOCUMENT TYPE: Patent
IT **1781-10-8** **1781-18-6** **1781-19-7**
1781-20-0 **1781-21-1** **3758-26-7**
3758-28-9 **3764-04-3** **3764-09-8**
RN 1781-10-8 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propyl- (7CI, 8CI) (CA INDEX NAME)



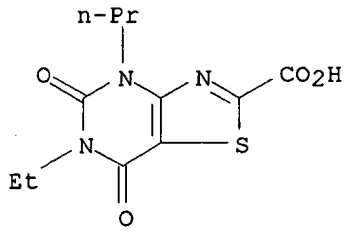
RN 1781-18-6 CAOLD
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 4,6-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



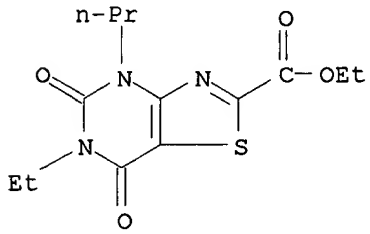
RN 1781-19-7 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxylic acid, 4,5,6,7-tetrahydro-4,6-dimethyl-5,7-dioxo- (7CI, 8CI) (CA INDEX NAME)



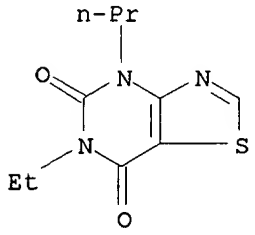
RN 1781-20-0 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxylic acid, 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propyl- (7CI, 8CI) (CA INDEX NAME)



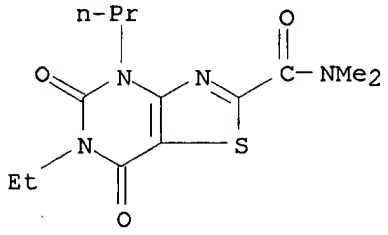
RN 1781-21-1 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxylic acid, 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



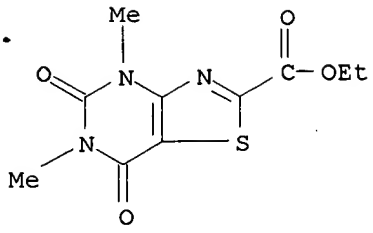
RN 3758-26-7 CAOLD
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 6-ethyl-4-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



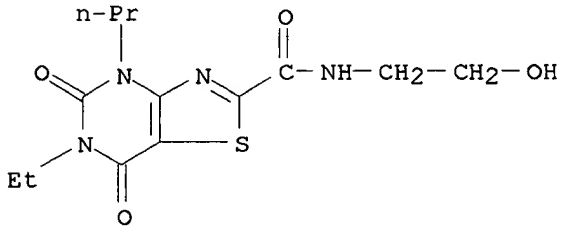
RN 3758-28-9 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-N,N-dimethyl-5,7-dioxo-4-propyl- (7CI, 8CI) (CA INDEX NAME)



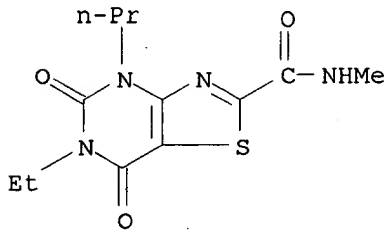
RN 3764-04-3 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxylic acid, 4,5,6,7-tetrahydro-4,6-dimethyl-5,7-dioxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



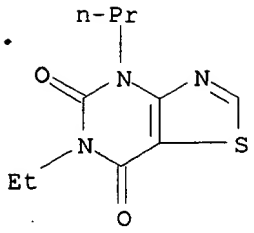
RN 3764-09-8 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-N-(2-hydroxyethyl)-5,7-dioxo-4-propyl- (7CI, 8CI) (CA INDEX NAME)



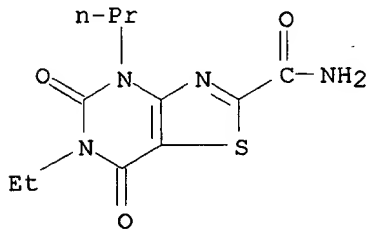
L7 ANSWER 2 OF 4 CAOLD COPYRIGHT 1999 ACS
ACCESSION NUMBER: CA62:4035h CAOLD
TITLE: phenothiazine derivs.
AUTHOR NAME: Boissier, Jacques R.; Malen, C.
DOCUMENT TYPE: Patent
TITLE: phenothiazine derivs.
PATENT ASSIGNEE: Societe Industrielle pour la Fabrication des Antibiotiques (S.I.F.A.)
DOCUMENT TYPE: Patent
IT **1781-11-9**
RN 1781-11-9 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-N-methyl-5,7-dioxo-4-propyl- (8CI) (CA INDEX NAME)



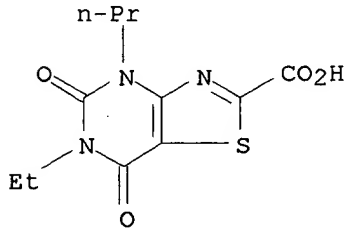
L7 ANSWER 3 OF 4 CAOLD COPYRIGHT 1999 ACS
ACCESSION NUMBER: CA57:8576a CAOLD
TITLE: bicyclic, cyclic, and acyclic azo compds.-2,3-diazabicyclo[2.2.2]-2-octene, 3,6-dimethyl-.DELTA.1-tetrahydropyridazine and azoisopropane
AUTHOR NAME: Cohen, Saul G.; Zand, R.
IT **3758-26-7**
RN 3758-26-7 CAOLD
CN Thiazolo[4,5-d]pyrimidine-5,7(4H,6H)-dione, 6-ethyl-4-propyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



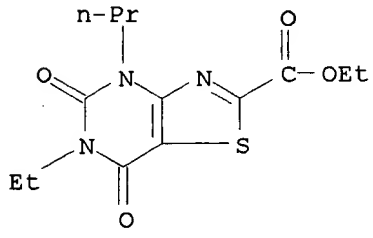
L7 ANSWER 4 OF 4 CAOLD COPYRIGHT 1999 ACS
ACCESSION NUMBER: CA57:8574c CAOLD
TITLE: rearrangement of sulfoxides of pyrimido [5,4-b][1,4]thiazines
AUTHOR NAME: Schroeder, Elmer F.; Dodson, R. M.
IT **1781-10-8 1781-20-0 1781-21-1**
3758-28-9 3764-09-8 95389-27-8
RN 1781-10-8 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propyl- (7CI, 8CI) (CA INDEX NAME)



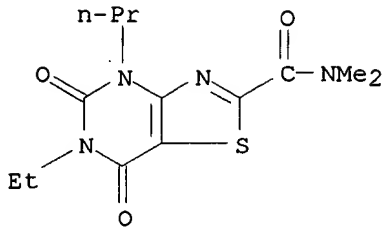
RN 1781-20-0 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxylic acid, 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propyl- (7CI, 8CI) (CA INDEX NAME)



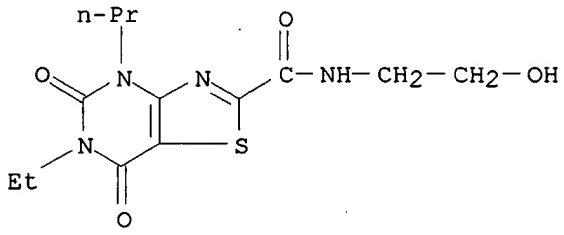
RN 1781-21-1 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxylic acid, 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propyl-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



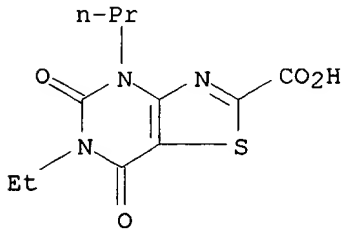
RN 3758-28-9 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-N,N-dimethyl-5,7-dioxo-4-propyl- (7CI, 8CI) (CA INDEX NAME)



RN 3764-09-8 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxamide, 6-ethyl-4,5,6,7-tetrahydro-N-(2-hydroxyethyl)-5,7-dioxo-4-propyl- (7CI, 8CI) (CA INDEX NAME)



RN 95389-27-8 CAOLD
CN Thiazolo[4,5-d]pyrimidine-2-carboxylic acid, 6-ethyl-4,5,6,7-tetrahydro-5,7-dioxo-4-propyl-, hydrate (7CI) (CA INDEX NAME)



● H_2O